Good luck on your enterprise.

May I suggest a sub-problem with which you will have to grapple anyhow, and will help you stage your work?

This is to "canonicate" a chemical graph. The procedure accepts as input a description of a specific structure in arbitrary form, and outputs one in accordance with the canons of Dendral order. This is a vital part of the structure-generator, but does not yet require a lot of book-keeping detail needed for stepping from one to the next radical in sequence. Please do not hesitate to

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let me know of your problems + successes.